Continuum HFB calculations with finite range pairing interactions

M. Grasso,[1] N. Van Giai,[1] N. Sandulescu,[2,3]
[1] *Institut de Physique Nucléaire, IN2P3-CNRS, Université Paris-Sud, 91406 Orsay Cedex, France*
[2] *Institute for Physics and Nuclear Engineering, P.O. Box MG-6, 76900 Bucharest, Romania*
[3] *Research Center For Nuclear Physics, Osaka University, Ibaraki, Osaka, 567-0047, Japan*

Abstract

A new method of calculating pairing correlations in coordinate space with finite range interactions is presented. In the Hartree-Fock-Bogoliubov (HFB) approach the mean field part is derived from a Skyrme-type force whereas the pairing field is constructed with a Gogny force. An iterative scheme is used for solving the integro-differential HFB equations via the introduction of a local equivalent potential. The method is illustrated on the case of the nucleus ^{18}C. It is shown that the results are insensitive to the cut off value in the quasiparticle spectrum if this value is above 100 MeV.

The treatment of pairing correlations is very important for the description of the properties of weakly bound nuclei situated close to the drip lines. The Hartree-Fock-Bogoliubov (HFB) method [1] is the the commonly adopted approach for treating self-consistently both the mean field contributions and the pairing correlations. Various effective interactions are available and can be used in the mean field and pairing channels of the HFB equations. They are of two types, namely zero-range forces [2–6] and finite range forces whose typical representatives are the Gogny forces [7].

Zero-range forces are widely used because the self-consistent equations can be conveniently solved in coordinate space. In loosely bound systems such as unstable nuclei, continuum effects in the pairing channel become important since their Fermi energies are typically close to zero and the pairing correlations can easily populate the continuum. Then, working in coordinate space is an advantage because the continuum effects can be accurately treated [8,9]. On the other hand, a zero-range pairing interaction has the well-known pathology of producing diverging contributions if no cut off is imposed on the quasiparticle space. This cut off must be an inherent part of the phenomenological zero-range interaction [10], but it is not clear which cut off value must be adopted for a given interaction and a given nucleus. We note that some regularization scheme has been proposed recently [11] for dealing with the question of HFB equations with zero-range pairing interactions.

Finite range pairing interactions of course do not require in principle a truncation of the quasiparticle space, even though in practical calculations the summations are restricted to quasiparticle energies below some cut off energy $E_{c.o.}$. If $E_{c.o.}$ is large enough the results no longer depend on its precise value, in contrast to the case of zero-range interactions. It is desirable therefore to have a method which combines the advantages of solving HFB equations in coordinate space and of describing pairing correlations with a finite range interaction. It is the purpose of this paper to propose such a method and to illustrate it by comparing results obtained with Skyrme and Gogny interactions.

We treat the continuum states exactly as explained in Ref. [9] where Skyrme-type interactions were used both in the mean field and pairing channels. Here, we keep a Skyrme force for the Hartree-Fock (HF) mean field but the pairing interaction is taken as a Gogny force. The calculations are done for the neutron-rich nucleus ^{18}C with the Skyrme interaction SLy4 [6] in the mean field channel and the Gogny interaction D1S [12] in the pairing channel.

For clarity we recall the general form of the coupled integro-differential HFB equations in coordinate representation [8]:

$$\int d^3\mathbf{r}' \sum_{\sigma'} \begin{pmatrix} h(\mathbf{r}\sigma,\mathbf{r}'\sigma') & \tilde{h}(\mathbf{r}\sigma,\mathbf{r}'\sigma' \\ \tilde{h}(\mathbf{r}\sigma,\mathbf{r}'\sigma') & -h(\mathbf{r}\sigma,\mathbf{r}'\sigma' \end{pmatrix} \begin{pmatrix} \phi_1(E,\mathbf{r}'\sigma') \\ \phi_2(E,\mathbf{r}'\sigma') \end{pmatrix} = \begin{pmatrix} E+E_F & 0 \\ 0 & E-E_F \end{pmatrix} \begin{pmatrix} \phi_1(E,\mathbf{r}\sigma) \\ \phi_2(E,\mathbf{r}\sigma) \end{pmatrix} , \tag{1}$$

where E_F is the Fermi energy, ϕ_1 and ϕ_2 are the upper and lower components of the HFB quasiparticle wave functions, respectively. In Eq.(1) the HF operator is a sum of kinetic and mean field components:

$$h(\mathbf{r}\sigma,\mathbf{r}'\sigma') = T(\mathbf{r},\mathbf{r}')\delta_{\sigma\sigma'} + \Gamma(\mathbf{r}\sigma,\mathbf{r}'\sigma') , \tag{2}$$

$$\Gamma(\mathbf{r}\sigma,\mathbf{r}'\sigma') = \int d^3\mathbf{r_1} d^3\mathbf{r_2} \sum_{\sigma_1\sigma_2} V(\mathbf{r}\sigma,\mathbf{r_1}\sigma_1;\mathbf{r}'\sigma',\mathbf{r_2}\sigma_2)\rho(\mathbf{r_2}\sigma_2,\mathbf{r_1}\sigma_1) . \tag{3}$$

When the HF interaction V is a Skyrme force, the mean field Γ is just a functional of the local particle density $\rho(\mathbf{r})$ and of its derivatives. Then, the HF operator h is a differential operator, which is a familiar property of Skyrme-HF models. On the other hand, the pairing interaction V_{pair} is a local force of finite range, and the pairing operator $\tilde{h}(\mathbf{r}\sigma,\mathbf{r}'\sigma')$ remains a fully non-local kernel obtained by folding V_{pair} with the pairing density $\tilde{\rho}$:

$$\tilde{h}(\mathbf{r}\sigma,\mathbf{r}'\sigma') = \int d^3\mathbf{r_1} d^3\mathbf{r_2} \sum_{\sigma_1\sigma_2} 2\sigma'\sigma_2' V_{pair}(\mathbf{r}\sigma,\mathbf{r}'-\sigma';\mathbf{r_1}\sigma_1,\mathbf{r_2}-\sigma_2)\tilde{\rho}(\mathbf{r_1}\sigma_1,\mathbf{r_2}\sigma_2) . \tag{4}$$

This is the new feature as compared to the equations discussed and solved in Refs. [8,9].

We choose to work with positive energy quasiparticle states, and the particle and pairing densities are expressed as:

$$\rho(\mathbf{r}\sigma,\mathbf{r}'\sigma) = \sum_{0<E_n<-E_F} \phi_2(E_n,\mathbf{r}\sigma)\phi_2^*(E_n,\mathbf{r}'\sigma) + \int_{-E_F}^{E_{c.o.}} dE\phi_2(E,\mathbf{r}\sigma)\phi_2^*(E,\mathbf{r}'\sigma) , \tag{5}$$

$$\tilde{\rho}(\mathbf{r}\sigma,\mathbf{r}'\sigma) = -\sum_{0<E_n<-E_F} \phi_2(E_n,\mathbf{r}\sigma)\phi_1^*(E_n,\mathbf{r}'\sigma) - \int_{-E_F}^{E_{c.o.}} dE\phi_2(E,\mathbf{r}\sigma)\phi_1^*(E,\mathbf{r}'\sigma) . \tag{6}$$

In Eqs. (5) and (6) the summations are over the discrete states that are situated in the region of the spectrum $0 < E_n < -E_F$ whereas the integrals run over the continuum part of the spectrum up to a chosen cut off.

We now take for V_{pair} a Gogny force which contains a sum of two gaussians, a zero-range density-dependent part and a zero-range spin-orbit part. Within the parametrisation D1S [12] that we adopt in this work the zero-range density-dependent part does not contribute. Let us explain the contribution of the gaussian terms. That of the spin-orbit part is also included in the calculations presented below although its effect is quite small. The finite range part of the interaction is:

$$V_{pair}(\mathbf{r_1}-\mathbf{r_2}) = \sum_{\alpha=1,2} (W_\alpha + B_\alpha \mathbf{P}_\sigma - H_\alpha \mathbf{P}_\tau - M_\alpha \mathbf{P}_\sigma \mathbf{P}_\tau) e^{\frac{-|\mathbf{r_1}-\mathbf{r_2}|^2}{\mu_\alpha^2}} , \tag{7}$$

where W_α, B_α, H_α, M_α and μ_α are parameters, $\mathbf{P}_\sigma$ and $\mathbf{P}_\tau$ are the spin and isospin exchange operators, respectively. Then, the pairing operator (4) becomes [10]:

$$\tilde{h}(\mathbf{r}\sigma, \mathbf{r}'\sigma) = \sum_{\alpha=1,2} e^{\frac{-|\mathbf{r}-\mathbf{r}'|^2}{\mu_\alpha^2}} \left[(W_\alpha - H_\alpha)\tilde{\rho}(\mathbf{r}\sigma, \mathbf{r}'\sigma) - (B_\alpha - M_\alpha)\tilde{\rho}(\mathbf{r}'\sigma, \mathbf{r}\sigma)\right] . \tag{8}$$

In the following we will need the multipole expansions of the gaussian form factors:

$$e^{\frac{-|\mathbf{r}-\mathbf{r}'|^2}{\mu_\alpha^2}} = \sum_{LM} F_L^\alpha(r, r') Y_{LM}(\hat{r}) Y_{LM}^*(\hat{r'}) . \tag{9}$$

We restrict ourselves to the case of spherical symmetry, for simplicity. Then, the general set of equations (1) can be solved for each partial wave (l, j) separately. We define the radial parts of the quasiparticle wave functions $\Phi_i(E, \mathbf{r}\sigma)$ (i=1,2) by:

$$\Phi_i(Eljm, \mathbf{r}\sigma) = \frac{u_i(Elj, r)}{r} Y_{lm_l}(\hat{r})(lm_l \frac{1}{2}\sigma|jm)\chi(\sigma) , \tag{10}$$

where $\chi(\sigma)$ is a spinor corresponding to a spin projection σ. With the help of the definition (10) and the expansion (9) it is straightforward to obtain the multipole decomposition of the pairing field $\tilde{h}(\mathbf{r}, \mathbf{r}') \equiv \sum_\sigma \tilde{h}(\mathbf{r}\sigma, \mathbf{r}'\sigma)$:

$$\tilde{h}(\mathbf{r}, \mathbf{r}') = \sum_{L_1 M_1} \tilde{h}_{L_1}(r, r') Y_{L_1 M_1}(\hat{r}) Y_{L_1 M_1}^*(\hat{r'}) , \tag{11}$$

where

$$\begin{gathered} \tilde{h}_{L_1}(r, r') = \textstyle\sum_{\alpha=1,2} \sum_L F_L^\alpha(r, r') \frac{2L+1}{4\pi} \sum_{nlj} (2j+1) \\ \left[(H_\alpha - W_\alpha) \frac{u_2(nlj,r)}{r} \frac{u_1(nlj,r')}{r'} - (M_\alpha - B_\alpha) \frac{u_2(nlj,r')}{r'} \frac{u_1(nlj,r)}{r}\right] \\ \begin{pmatrix} L & l & L_1 \\ 0 & 0 & 0 \end{pmatrix}^2 . \end{gathered} \tag{12}$$

The summations over n in Eq. (12) become integrals over the energy for the continuum states.

For each partial wave (lj) one has to solve a system of two coupled integro-differential equations whose general structure is:

$$hu_1(r) + \int \tilde{h}(r,r')u_2(r')r'^2dr' = (E+E_F)u_1(r) \ ,$$
$$\int \tilde{h}(r,r')u_1(r')r'^2dr' - hu_2(r) = (E-E_F)u_2(r) \ . \tag{13}$$

In the context of HF equations with finite range interactions it has been shown by Vautherin and Vénéroni [13] that one can transform the HF integro-differential equation into a purely differential equation by introducing a so-called trivially equivalent local potential. Here, we generalize this method to the system of equations (13) by defining local equivalent potentials $U_i(r)$ in the following way:

$$\int \tilde{h}(r,r')u_i(r')r'^2dr' = \frac{1}{u_i(r)}(\int \tilde{h}(r,r')u_i(r')r'^2dr')u_i(r)$$
$$\equiv U_i(r)u_i(r) \ , \ i=1,2 \ . \tag{14}$$

Then, Eqs.(13) become formally a system of two coupled differential equations where the potentials depend on the solutions and therefore they must be solved iteratively. This is not a major problem since the self-consistency requirement already leads to an iterative scheme.

An additional difficulty comes from the fact that the local potentials $U_i(r)$ have poles at the nodes of the wave functions $u_i(r)$. In Ref. [13] a very simple and efficient method was proposed to overcome this problem, based on the linearization of the local equivalent potential around the poles. Another equivalent potential $U_i(\epsilon,r)$ is introduced; it is equal to $U_i(r)$ everywhere except inside the intervals $[r_0-\epsilon, r_0+\epsilon]$ where r_0 denotes a pole of $U_i(r)$. Inside these intervals $U_i(\epsilon,r)$ is chosen as a segment which joins the values of $U_i(r_0-\epsilon)$ and $U_i(r_0+\epsilon)$. The approximation is good if ϵ is small enough not to wash out the shape of the potential. Thus, $U_i(r)$ is replaced by the following potential:

$$U_i^{(n+1)}(\epsilon_{n+1},r) = R_{\epsilon_{n+1}}\left\{\frac{1}{u_i^{(n)}(r)}\int r'^2dr'\tilde{h}(r,r')u_i(r')^{(n)}dr'\right\} \ , \tag{15}$$

where $R_{\epsilon_{n+1}}$ indicates the linear interpolation procedure described above and n counts the iterations by which the HFB equations are solved. The parameter ϵ depends on the iteration and it is chosen so that $lim \ \epsilon_n = 0$. At each iteration of the HFB scheme we evaluate the equivalent potentials of all quasiparticle states by using the wave functions of the previous iteration and we repeat this procedure until convergence.

We compare now the HFB results for ^{18}C obtained by using in the pairing channel either the finite range Gogny interaction D1S or a zero-range interaction. In both cases the Skyrme interaction SLy4 is used to construct the mean field. The quasiparticle continuum is fully treated (no box boundary conditions) as described in Ref. [9]. As it was said before, the problem with the use of a zero-range pairing interaction is the divergence of the pairing correlations when one increases the cut off energy $E_{c.o.}$. This is illustrated in Fig.1 where the particle (top) and pairing (bottom) densities of neutrons in ^{18}C are plotted. The zero-range pairing interaction in this case is [10]:

$$V_{pair}(\mathbf{r},\mathbf{r}') = V_0\delta(\mathbf{r}-\mathbf{r}')\left[1-\left(\frac{\rho(\mathbf{r})}{\rho_C}\right)^\gamma\right] \ , \tag{16}$$

where $\rho(\mathbf{r})$ is the particle density, and the values of V_0 and γ are deduced from the parameters of SLy4 (V_0=-2488.9 MeV fm^3, γ=1/6, with the choice $\rho_C = 0.133$ fm^{-3}). Different densities corresponding to different values of $E_{c.o.}$ are plotted. We can observe that, while the particle density is almost stable with respect to the cut off energy the pairing density increases with $E_{c.o.}$ as it is expected. This indicates that the mean field properties are not much affected by the enlarging of the continuum phase space while the pairing properties are very sensitive to it. If one moves the cut off towards higher values the pairing density continues to increase and it never converges to a stable result. This problem is eliminated when a finite range interaction is used to construct the pairing field.

We show in the upper part of Fig.2 the total energies of ^{18}C calculated with the two pairing interactions and for cut off values ranging from 70 MeV up to 120 MeV. We observe that the system is more and more bound when the cutoff increases; this is due to the fact that pairing correlations become more and more important. While in the case of the zero-range interaction the total energy continues to decrease in the chosen interval of cut off values, in the case of the Gogny interaction the total energy converges and reaches a stable value equal to -130.65 MeV at a cut off of 100 MeV. We can equivalently observe this convergence of the energy by studying the trend of the pairing correlation energies which are shown in the lower part of Fig. 2 for the same cut off values. The pairing correlation energy is defined as follows:

$$E_P \equiv E(HF) - E(HFB) \ , \tag{17}$$

where E indicates the total energy of the nucleus. The quantity E_P is the difference in the total binding energies between the HF and HFB calculations; thus, it gives an estimation of the amount of pairing correlations. In the figure one can observe that these energies always increase for the zero-range interaction indicating the increasing of the amount of pairing correlations while they reach a stable value equal to 16.04 MeV for the Gogny interaction. It is easy to understand why the results with the latter interaction become stable for cut off energies around 100 MeV or beyond. The shortest range of the two gaussian form factors is 0.7 fm, which corresponds to 2.86 fm^{-1} in momentum space, i.e., a kinetic energy of about 160 MeV. The depth of the mean field potential being about 40 MeV one can estimate that this kinetic energy corresponds to a quasiparticle energy around 120 MeV.

Another quantity that one can study as a function of the cut off energy is the mean square radius of the pairing density. Indeed, the mean square radius of the particle density must be stable against $E_{c.o.}$ because the $u_2^2(r)$ functions entering Eq.(5) are negligible for large quasiparticle energies. In contrast, the $u_1(r)u_2(r)$ factors of Eq.(6) do not decrease so fast with increasing quasiparticle energies. Let us define:

$$\langle r^\alpha \rangle \equiv \int r^2 dr \tilde{\rho}(r) r^\alpha \ . \tag{18}$$

In Fig. 3 we show $\langle r^2 \rangle$ for the two pairing interactions. Again, while $\langle r^2 \rangle$ always increases in the case of the zero-range interaction it reaches a stable value of about 34.5 fm^2 at a cut off of 95 MeV in the case of the Gogny interaction. This convergence indicates that the pairing density does not change when the cut off is moved beyond the value of 95 MeV.

In this work we have presented a new method for solving HFB equations in coordinate space with finite range pairing interactions. This may be useful in systems where the chemical potential is close to zero and an accurate treatment of the quasiparticle continuum is required. As an illustration of the method we have solved the HFB equations for a neutron-rich nucleus, using the finite range force D1S as pairing interaction. Because our main purpose here is to discuss the respective behaviour of zero-range and finite range interactions in the pairing channel, we have kept in the present application the Skyrme-type force SLy4 to generate the HF mean field. A further step toward full self-consistency with the same finite range force for calculating the mean field and the pairing field can be made, using the same technique of local equivalent potential also for the mean field as it was already done in the HF context [13]. Work in this direction is in progress.

The authors wish to thank P.F. Bortignon, P. Schuck and N. Vinh Mau for fruitful discussions. One of us (M.G.) is a recipient of a European Community Marie Curie Fellowship. Two of us (N.V.G. and N.S.) acknowledge that this work was done in the framework of IN2P3(France)-IPNE(Romania) Collaboration.

REFERENCES

[1] P. Ring and P. Schuck, *The Nuclear Many-Body Problem* (Springer-Verlag, Berlin, 1980).

[2] T.H.R. Skyrme, Phil. Mag. **1**, 1043 (1956), T.H.R. Skyrme, Nucl. Phys. **9**, 615, 635 (1959).

[3] D.G. Vautherin and D.M. Brink, Phys. Rev. **C 5**, 626 (1972).

[4] M. Beiner, H. Flocard, N.V. Giai, and P. Quentin, Nucl. Phys. **A 238**, 29 (1975).

[5] N. Van Giai and H. Sagawa, Nucl. Phys. **A 371**, 1 (1981).

[6] E. Chabanat, et al., Nucl. Phys. **A 635**, 231 (1998).

[7] J. Dechargé and D. Gogny, Phys. Rev. **C 21**, 1568 (1980).

[8] J. Dobaczewski, H. Flocard, and J. Treiner, Nucl. Phys. **A 422**, 103 (1984).

[9] M. Grasso, N. Sandulescu, Nguyen Van Giai, R.J. Liotta, Phys. Rev. **C 64**, 064321 (2001).

[10] J. Dobaczewzki, W. Nazarewicz, T.R. Werner, J.-F. Berger, C.R. Chinn, and J. Dechargé, Phys. Rev. **C 53**, 2809 (1996).

[11] A. Bulgac and Y. Yu, nucl-th/0106062, A. Bulgac, nucl-th/0108014.

[12] L.M. Robledo, J.L. Egido, J.-F. Berger, and M. Girod, Phys. Lett. **B 187**, 223 (1987).

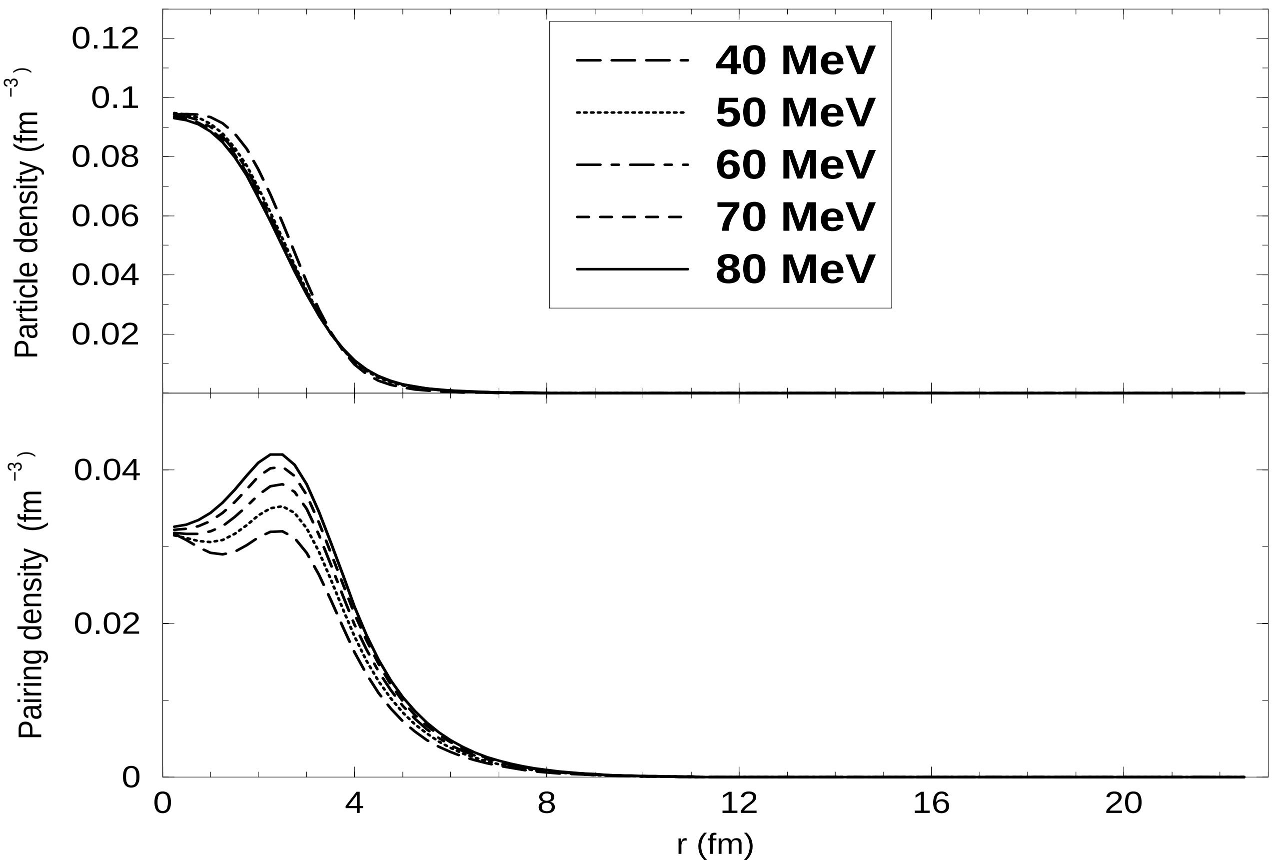
[13] D.G. Vautherin and M. Veneroni, Phys. Lett. **B 25**, 175 (1967).

FIGURES

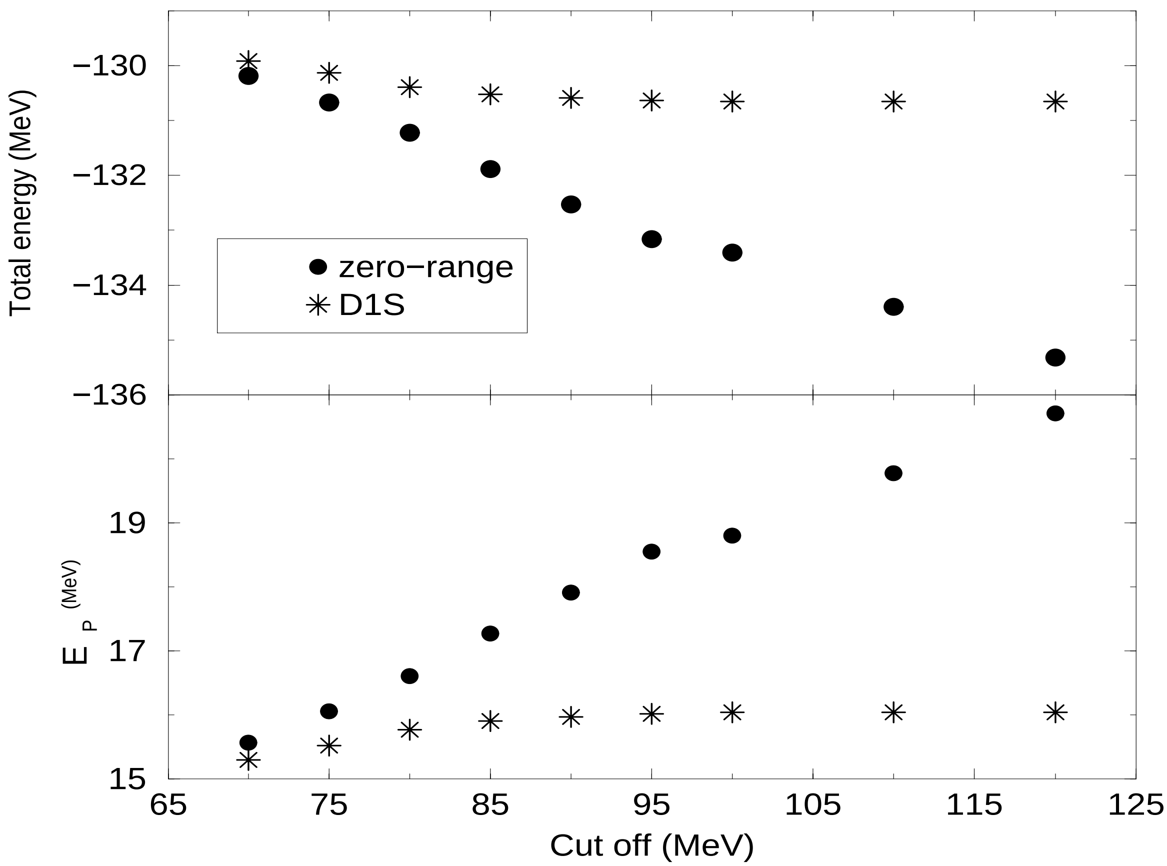
FIG. 1. Neutron particle (top) and pairing (bottom) densities of ^{18}C obtained with the zero-range pairing interaction, Eq. (16), for different values of the cut off.

FIG. 2. Upper part: Total energies of ^{18}C obtained with zero-range and Gogny pairing interactions for different cut off values. Lower part: Pairing correlation energies, Eq. (17), obtained with zero-range (circles) and Gogny (stars) pairing interactions for different cut off values for ^{18}C.

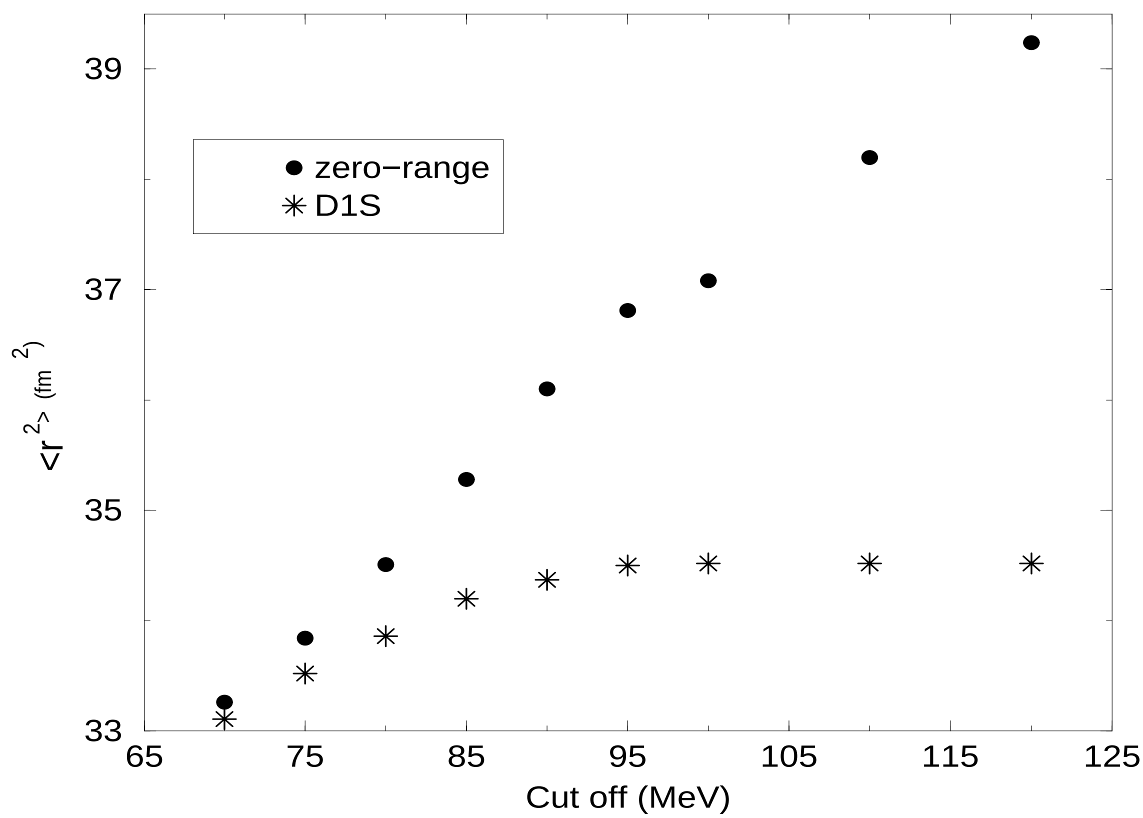
FIG. 3. Mean square radii of pairing densities, Eq. (18), obtained with zero-range (circles) and Gogny (stars) pairing interactions for different cut off values for ^{18}C.



40 MeV
50 MeV
60 MeV
70 MeV
80 MeV
Particle density (fm $^{-3}$)
0.12
0.1
0.08
0.06
0.04
0.02
Pairing density (fm $^{-3}$)
0.04
0.02
0
0
4
8
12
16
20
r (fm)



Total energy (MeV)
−130
−132
−134
−136
zero−range
D1S
E P (MeV)
19
17
15
65
75
85
95
105
115
125
Cut off (MeV)


zero−range
D1S
39
37
35
33
65
75
85
95
105
115
125
Cut off (MeV)
<r^2> (fm ^{2})